Development of Computer-Aided Design Tools for Automotive Batteries

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General Motors R&D Center

Date: May 15, 2012

Project ID # ES119

Overview

Timeline

- Start – June 2011
- Finish – May 2014
- 20% Complete

Budget

- Total project funding: $7.2 M
  - —DOE - $ 3,600 K
  - —Contractor – $ 3,600 K
- Funding received in FY11
  - —$ 369 K
- No funding change

Barriers

- Barriers
  a) Material properties and cell structures are proprietary and difficult to obtain
  b) Complexity of multi-scale, multi-physics interactions
- Targets -shorten time and cost for design and development of EDV battery systems

Partners

- GM : End user requirements, verification/validation, project management
- ANSYS : Software development
- ESim : Cell level sub models, life model
- NREL : Technical monitor

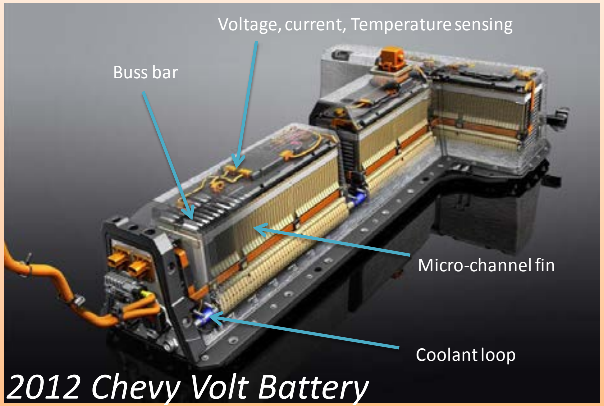
Project Lead: GM R&D Center

Funding provided by Dave Howell of the DOE Vehicle Technologies Program . The activity is managed by Brian Cunningham of Vehicle Technologies. Subcontracted by NREL, Gi-Heon Kim Technical Monitor

Development of Computer-Aided Design Tools for Automotive Batteries (CAEBAT)

Project Objectives - Support of DOE CAEBAT

The automotive industry requires CAE design tools that include the following capabilities.

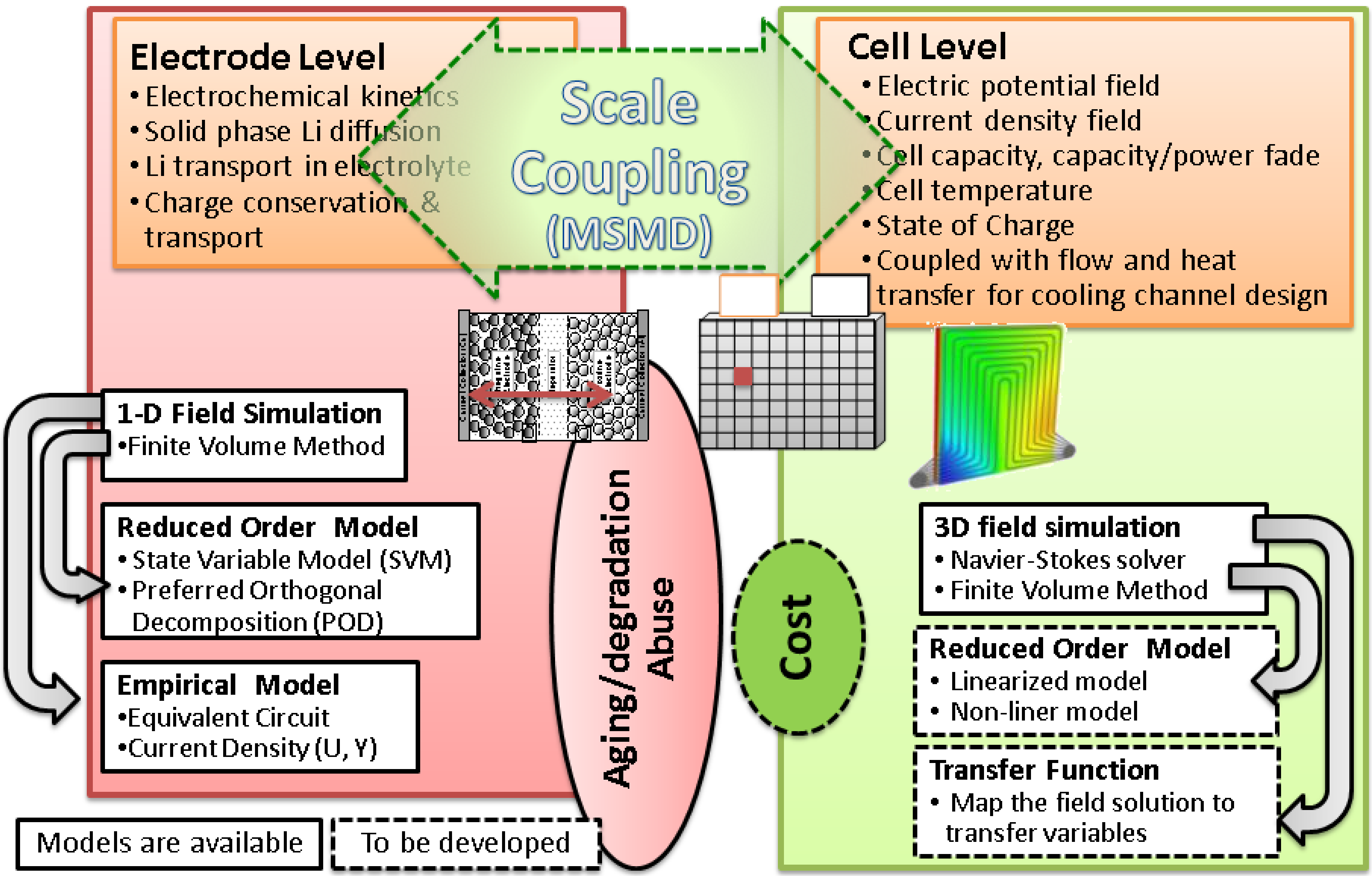


- **Address Multi-Scale Physics Interactions:**
  - Integrate physics and chemistry in a computationally efficient manner.
- **Provide Flexibilities:**
  - Provide a platform to enable various simulation strategies.
- **Provide Expandable Framework:**
  - Enable future users to easily add new physics of interest.
- **Verify and Validate Models:**
  - Ensure model predictions agree with experimental data by performing carefully designed experiments.

Milestones

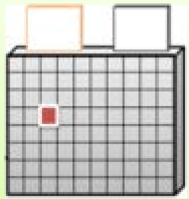
Month /Year	Milestone or Go/No-Go Decision	
June-2012	Go/No-Go decision: Define end user requirements for the cell level and the pack level design tools. The cell level model includes three sub models that covers the particle and electrode level (P2D), Semi-empirical cell level model (NTGK), and equivalent circuit model (ECM). Demonstrate scale coupling of various sub models by MSMD approach for the cell level. Milestone: Deliver the first cell level model.	On track
June-2013	Milestone: Validation of the cell level model. Deliver the final cell level simulation tool. Deliver the first pack level model. The pack level model includes a system level co-simulation capability and reduced order models (ROM).	On track
June - 2014	Milestone: Validation of the pack level model. Develop CAE process automation for the pack level simulations. Deliver the final pack level design tools. Incorporate the Open Architecture Software interface to allow other sub models, material database, physical input parameters, and future sub models.	On track

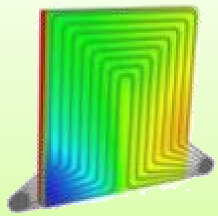
Approach for Cell Level



Approach for Pack Level Simulation

- Strategy is to offer a wide range of methods allowing analysts to trade off computational expense vs. resolution





Cell Level Model

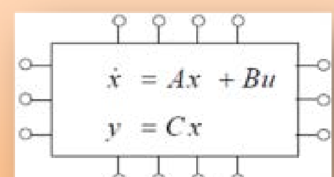
- Reduced Order Models for electrochemistry
- Cell level performance including local cooling channels

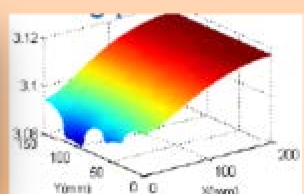
Pack Level Model

Co-simulation

Reduced-Order Models

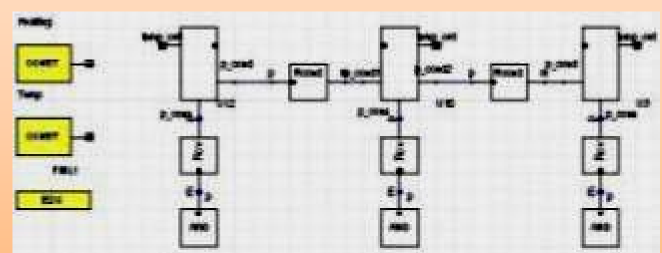
- Reduced order models for flow and thermal analysis at the pack level
- Reduced order cell models
- Ability to "expand" results



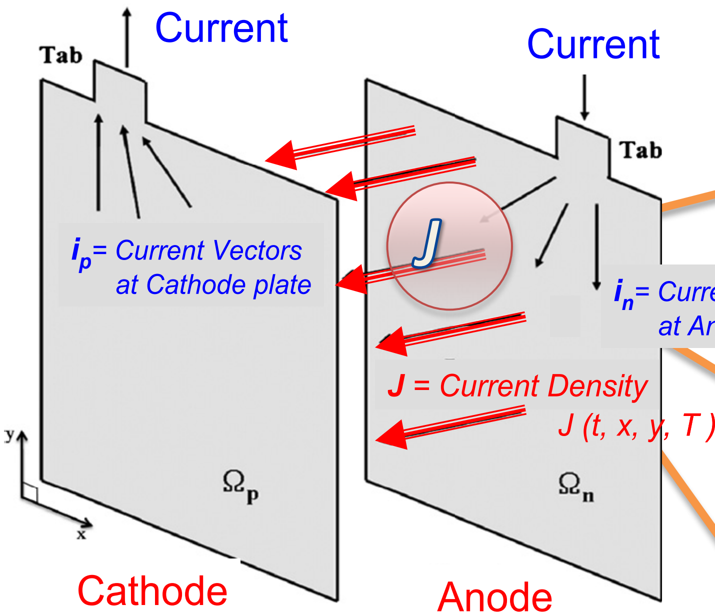


System Level Model

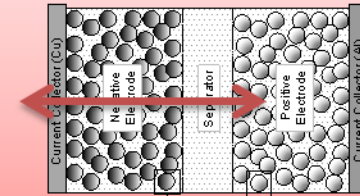
- Construct a "linear" or "non-linear" system simulation model from the full pack simulation model



Sub-models Integrated into the Cell



Newman, Li transport model (P2D)



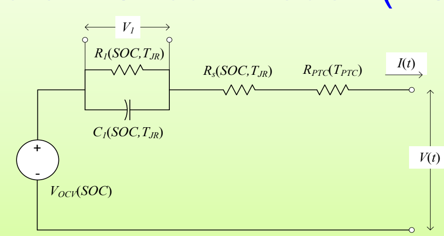
Newman, Tiedemann, Gu, Kim (NTGK)

$$J = Y(V_p - V_n - U)$$

$$U = f(DOD, T)$$

$$Y = g(DOD, T)$$

Equivalent Circuit Model (ECM)



- Electrochemical sub-models relate the local current density to the potential
- Cell model couples sub-models to thermal and electrical fields within the cell, integrates over multiple electrode-pairs

Cell Level Sub-models

	Model	Pros	Cons	Potential application area	Further development
P2D	Detailed electrochemistry modeling approach. Solve particle and electrode level including electrolyte	Potential to simulate local detail and cover wide range of cell chemistry	Many physical input parameters and material properties. Difficult to obtain these from the measurements.	Cell design	ROM. Need MSMD approach for cell level simulations
NTGK	Semi-empirical approach. 2 key functional parameters, U, Y. Solve electrical potential for the current collectors.	Practical 2-D approach. Non-uniform SOC, heat distribution	Unable to predict cell design changes without testing	Cell/Pack integration	Temperature effects. Transient terms. Aging, abuse conditions.
ECM	Empirical parameter fit from test data. Do not solve electric potential field.	Very simple. computationally very fast	Unable to predict cell design changes without testing	Pack optimization	Temperature effects.

Pack Level Strategies

	Model	Pros	Cons	Potential application area	Further development
Co-simulation	CFD-based cell models iteratively coupled to network/circuit pack model	Most accurate, no need for ROM-building, Earliest availability for testing	Computational cost (but can exploit periodicity, sampling, module hierarchy to improve over brute force approach)	Totally new designs, validation	Asynchronous time stepping, Automated user interface
Transient ROM	Build time-varying cell ROM from CFD, then use in pack-level simulation	Most efficient	Linearized about some particular values, e.g. coolant flow rate, state of health, etc.	Drive cycles, parametric studies	ROM algorithms, Storage, Results expansion
System level model	Construct system level models from the full pack simulation model.	Very fast and efficient	Solution available only at monitored locations. Requires full 3-D pack-level flow/thermal solution.	Battery management system, Drive cycles	Non-linearity due to variable flow rates

Overview of the first Cell Level Simulation Tool

Standard battery input parameters
- Geometry,
- Materials,
- Physical parameters,

Operating conditions
- Current (t)
- Voltage (t)
- Power (t)

Electrode sub-models
- P2D (Full)
- NTG semi-empirical
- ECM (equivalent circuit)

Build Interface for other sub-models

Other sub-models

Cell level tool

Cell level
- verification
- validation

Output
- Terminal V(t), I(t), P(t)
- Non-uniform Q
- SOC
- Cell temperature
- Coolant temperatures
-

The first cell level tool will includes 3 sub-models with a standard battery user interface and open interface for other sub-models. Cell level verification and validation will be performed after the first cell level tool is available.

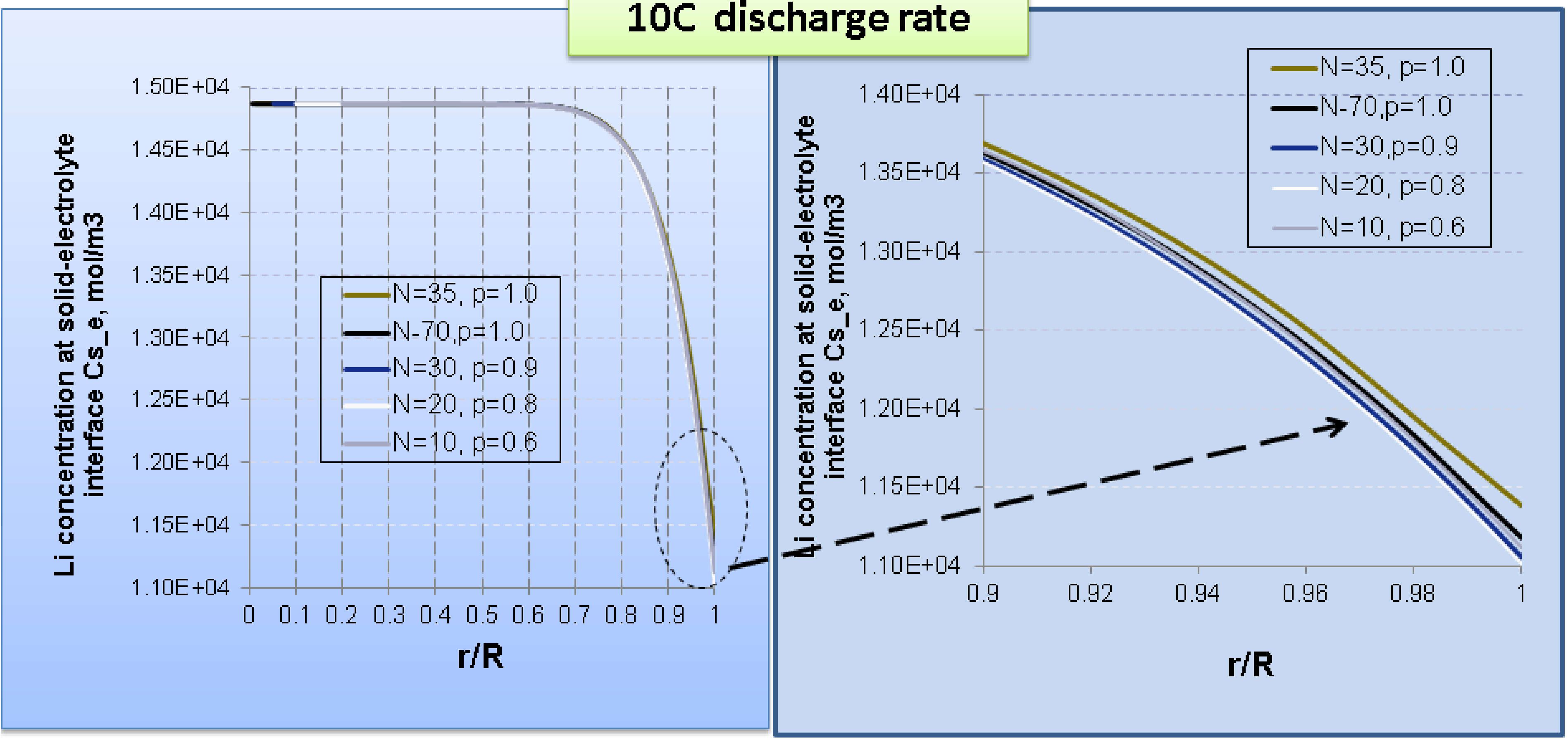
Technical accomplishments – Year 1

- End user needs have been defined for the cell level and the pack level design tools. Battery manufacturer's requirements has been obtained from LG Chem.
- Survey of existing potential cell level models has been completed.
- All three cell-level approaches have been prototyped.
- Simplorer-FLUENT co-simulation feature has been prototyped.
- Initial research has been conducted on ROM methods.
- Scale coupling between particle, electrode, and cell levels has been tested based on MSMD approach.
- A test plan and procedure for collecting test data from production cells to validate the cell design tool has been completed.
- CAE capability matrix has been defined for pack level applications in automotive industry.
- Performed monthly progress reviews with NREL and quarterly reviews with NREL and DOE.

Researching Simulation Best-Practice

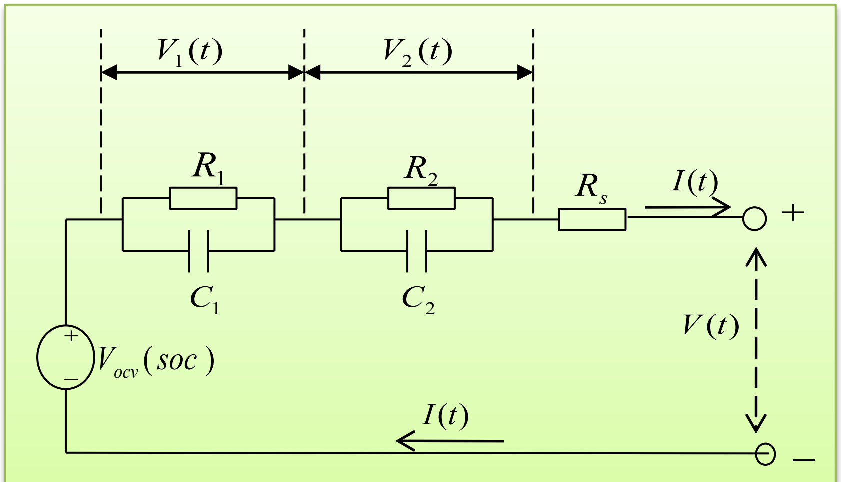
- P2D particle resolution study (non-uniform radial grid)
- Findings will be built into deliverables, providing automation for non-experts

10C discharge rate



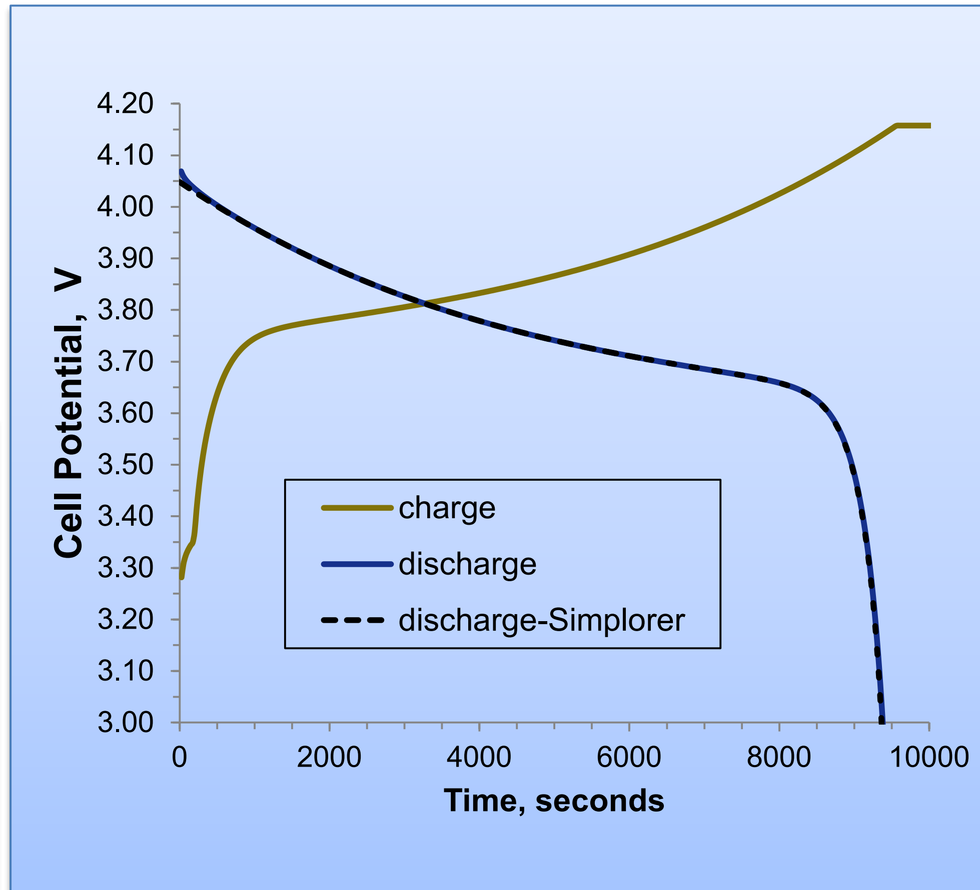
Equivalent Circuit Model implementation

ECM was implemented as a sub-model and validated with other results.



$$
\begin{cases}
V(t) = V_{OCV}(soc) + V_1 + V_2 - R_s(soc) I(t) \\
\dfrac{dV_1}{dt} = -\dfrac{1}{R_1(soc) C_1(soc)} V_1 - \dfrac{1}{C_1(soc)} I(t) \\
\dfrac{dV_2}{dt} = -\dfrac{1}{R_2(soc) C_2(soc)} V_2 - \dfrac{1}{C_2(soc)} I(t) \\
soc = soc_0 - \dfrac{\int_0^t I(t) dt}{3600 Q_{Ah}} \qquad I(t) = \begin{cases} > 0 & discharge \\ < 0 & charge \end{cases}
\end{cases}
$$

320 mA discharge/charge curves for a 850-mAh capacity cell



EC Model: Chen & Rincon-Mora (2006)

NTGK Model implementation

2D NTGK Model

$$\nabla^2 V_\mathrm{p} = -r_\mathrm{p} J \quad \text{in} \quad \Omega_\mathrm{p}$$

$$\nabla^2 V_\mathrm{n} = +r_\mathrm{n} J \quad \text{in} \quad \Omega_\mathrm{n}$$

Current Density Model

$$U = f(DOD, T)$$

$$Y = g(DOD, T)$$

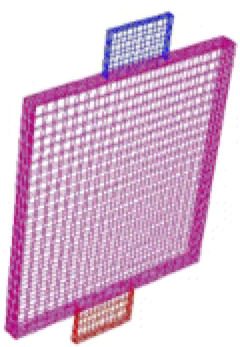
U and Y are fitting parameters depend on Depth of Discharge (DOD) and Temperature

3D MSMD Framework

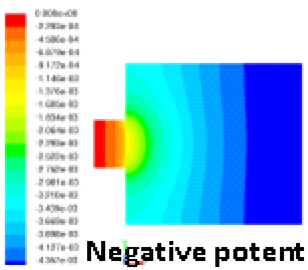
$$\nabla \cdot (\varepsilon_+ \sigma_+ \nabla \phi_+) = +aj$$

$$\nabla \cdot (\varepsilon_- \sigma_- \nabla \phi_-) = -aj$$

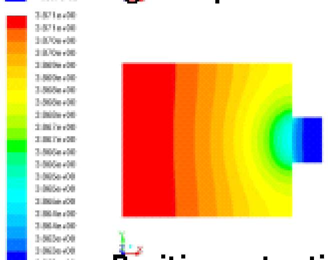
$$j = aY(\phi_+ - \phi_- - U) \quad A/m^3$$



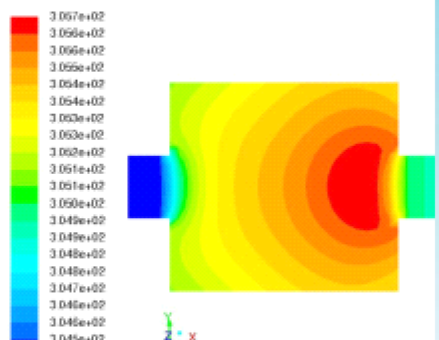
3-D Finite Volume



Negative potential

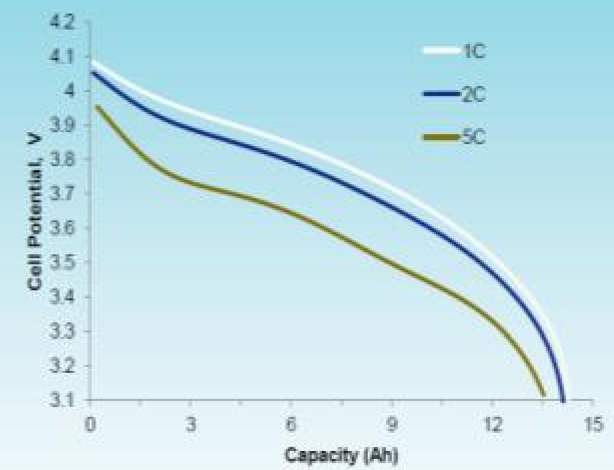


Positive potential



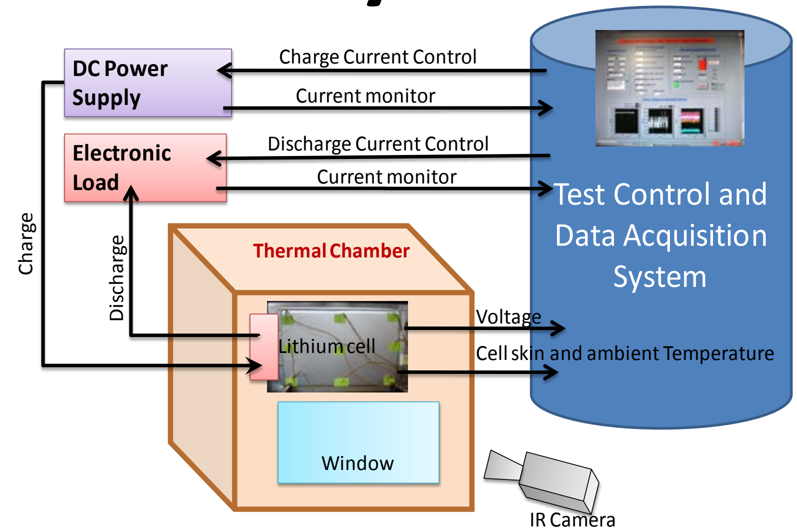
Temperature

- Discharge curve

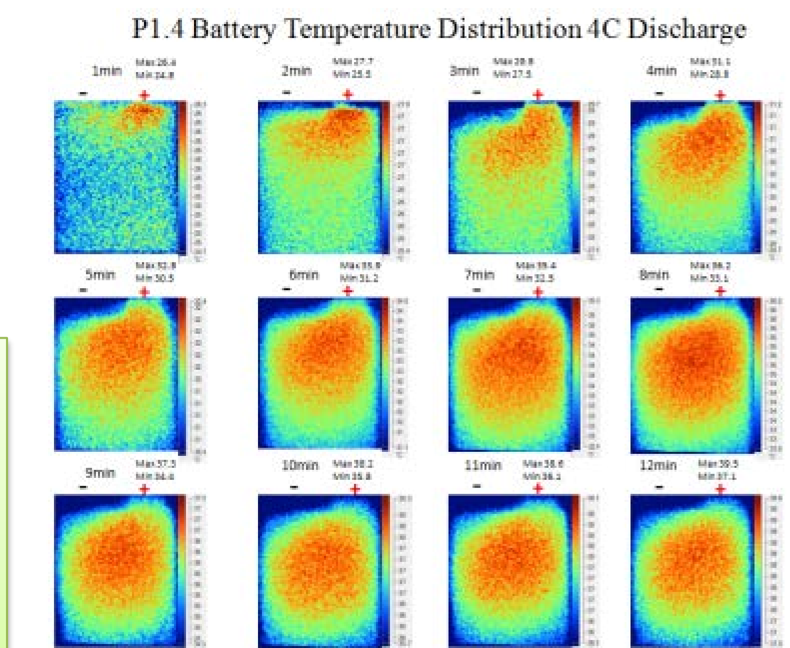


Cell Level Test & Validation by GM

Test	Test Conditions
Cell relaxation test	Environmental Temperature range: -20, -10, 0, 25, 40 Deg C C rate: 0.5C, 1C, 3C and 4C
Static capacity and HPPC test	Environmental Temperature range: 0, 10, 25, 40 Deg C
IR thermal imaging	10 to 90% SOC, room temperature, 1C, 3C and 4C
Cell cyclic life test	Environmental Temperature range: 0, 10, 25, 40 Deg C C rate: 2C, 3C SOC window: 30% to 90%
Cell Calorimeter	Same test condition cell cycling test



- Cell level validation test for electrical and thermal performance for the cell
- Thermocouple, thermal imaging, calorimeter test to measure the total heat generation and non-uniform heat source
- Cycle life test for aging model



Cell Cycle Life Test Procedure

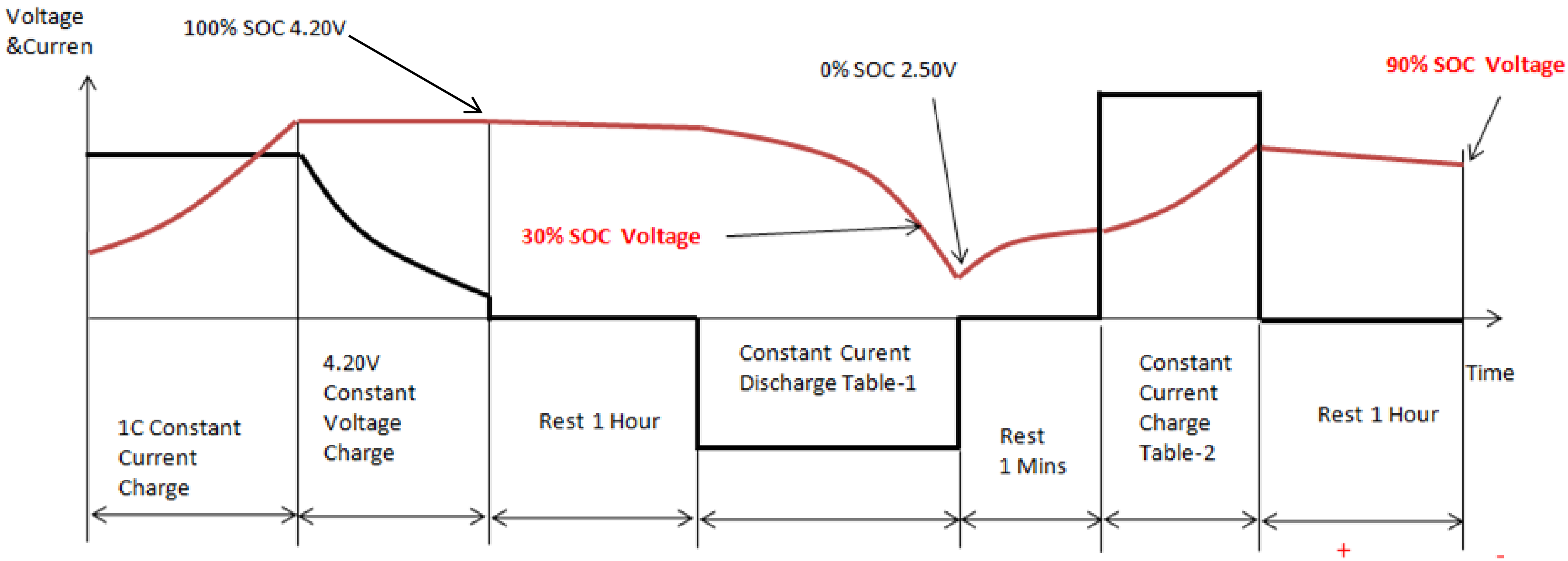


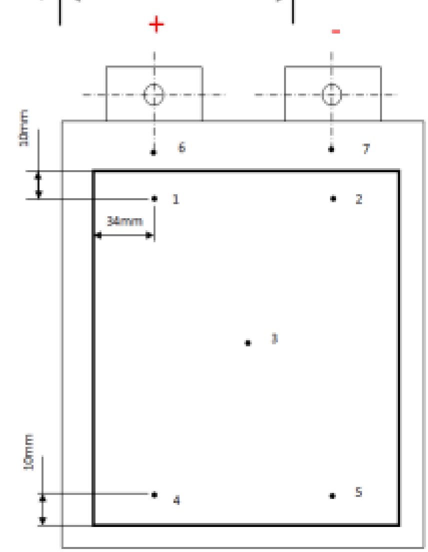
Table-1

Test	Parameter	Cycle Test Temperature			
		0°C	10°C	25°C	40°C
2C cycle	Disharge Current	30A	30A	30A	30A
3C Cycle	Disharge Current		45A	45A	45A

Table-2

Test	Parameter	Cycle Test Temperature			
		0°C	10°C	25°C	40°C
2C cycle	Charge Current	12A	20A	30A	30A
3C Cycle	Charge Current		20A	30A	30A

Test Cells in Thermal Chamber

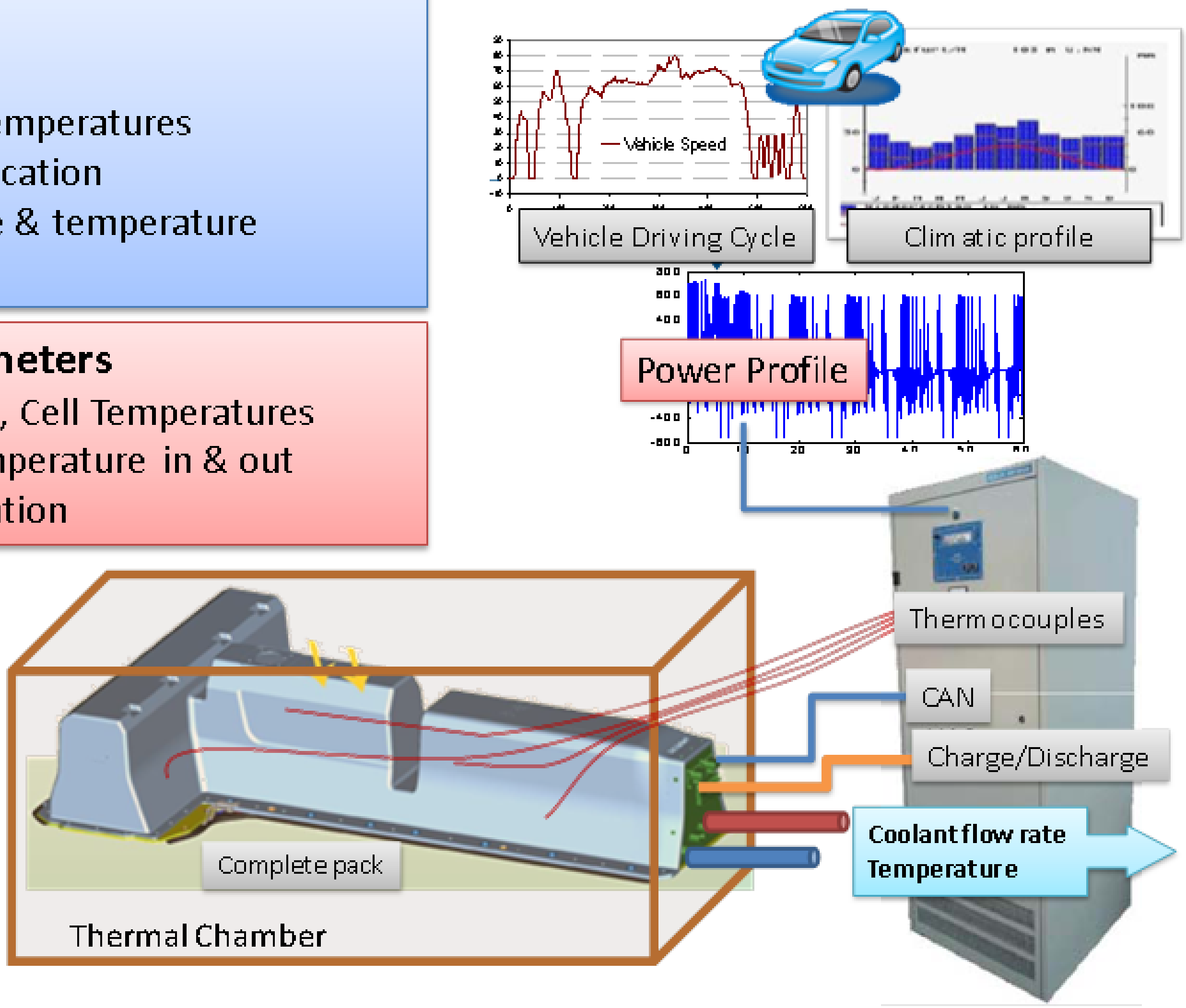


Temperature Monitor Point

Pack Level Validation

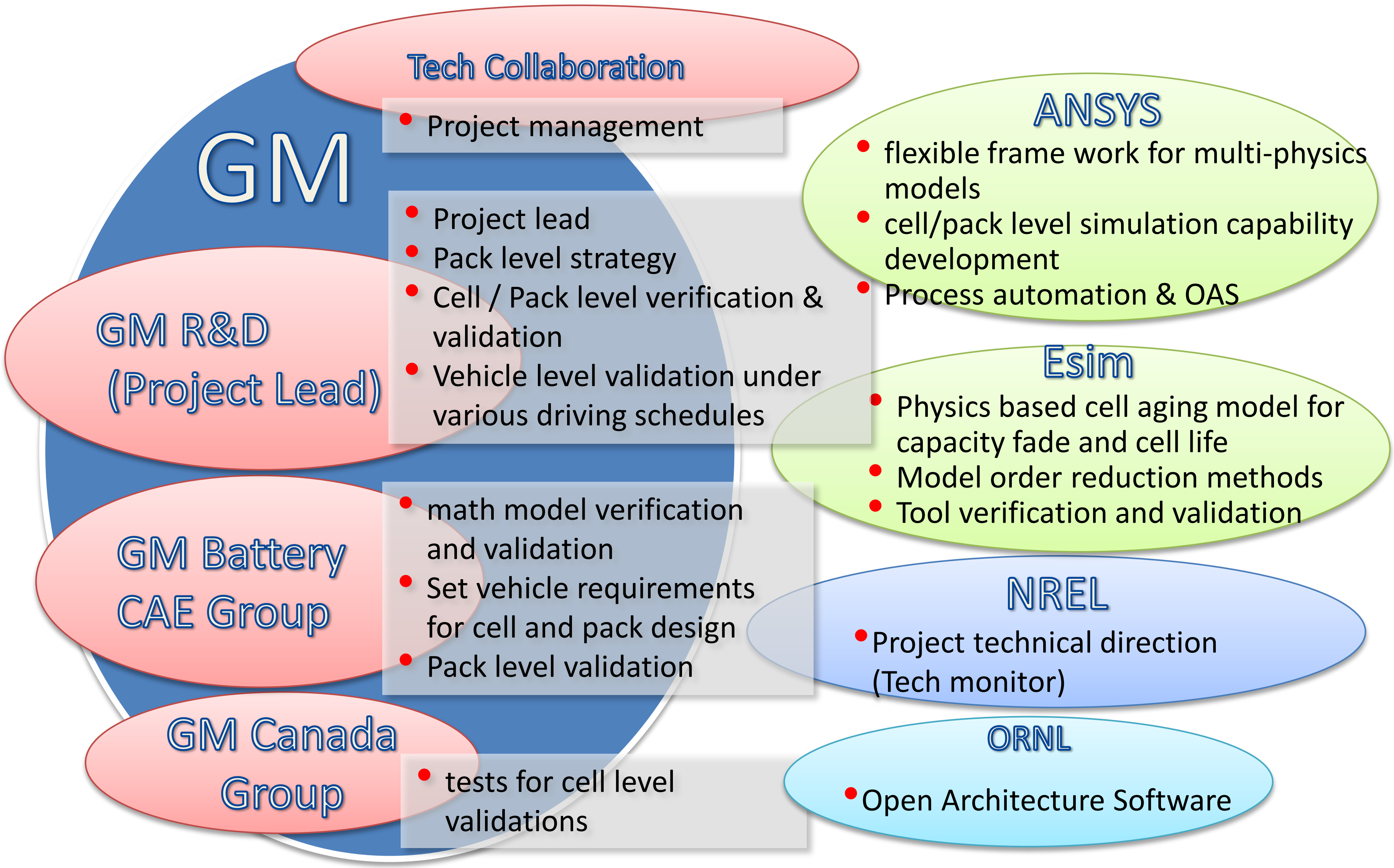
Pack level test
- Driving cycles
- Environmental temperatures
- Thermocouple location
- Coolant flow rate & temperature
- Cell chemistry

Validation Parameters
- SOC, Cell Voltage, Cell Temperatures
- Coolant flow Temperature in & out
- Total heat generation



♦ Pack level validation test data will be carefully selected from the existing GM battery Test database.

Collaborations



Future Work

- **Develop model order reduction methods for the pack level**
- **Extend cell-level models for aging and abuse**
- **Cell level verification and validation**
- **Pack level verification, validation, and demonstration**
  - ✓Define pack level validation requirements to meet the future capability matrix for pack level CAE performance.
  - ✓Identify suitable existing pack level test in progress or from previous tests (Liquid or Air cooling)performed in GM battery group.
  - ✓Build up the pack level simulation model including meshing and physical boundary conditions, operating conditions.
- **Develop battery-specific graphical user interface for workflow automation**
- **Build a standard data-exchange interface based on specifications from the OAS Workgroup**

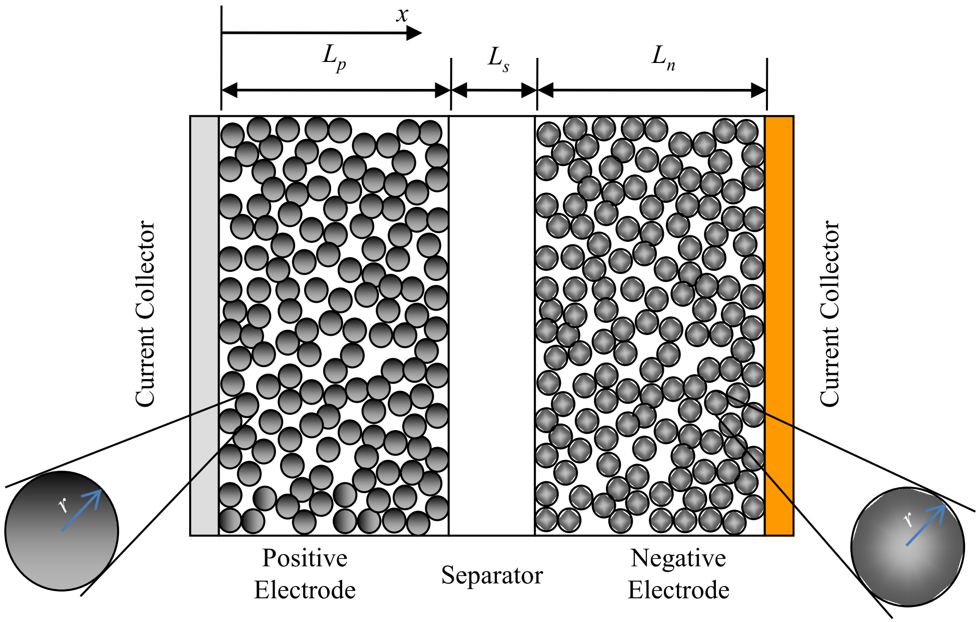
Summary

- **Overall project is on-track to meet all objectives, Year 1 technical progresses are consistent with the plan**
- **Cell level end user requirements have been defined and completed;**
  - ✓ Model inputs and outputs, geometry & meshing requirements, performance requirements. Standard input parameters were defined and shared with the OAS Work Group.
  - ✓ End user requirements from the battery manufacturer (LG Chem) was obtained . Other battery manufacturers are under consideration.
- **Cell level validation test in progress;**
  - ✓ Cell performance test in progress, cycle life test has been initiated.
  - ✓ Two different cell chemistries are chosen for validation (LG Chem, A123).
- **Pack level end user requirements have been defined and completed;**
  - ✓ CAE capability matrix, functionalities, user friendly features, acceptable accuracies and requirements for CPU time & turnaround time.
- **Principal remaining efforts and technical risks in the area of pack-level model;**
  - ✓ Various Pack level simulation strategies are under evaluation.

Technical Back-Up Slides

ESim LLC

Porous Electrode Lithium Ion Battery Model



- Positive Electrode

$$\frac{\partial c_{s,p}(r,t)}{\partial t}=D_{s,p}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_{s,p}(r,t)}{\partial r}\right)$$

$$\varepsilon_{\mathrm{p}}\frac{\partial c}{\partial t}=D_{\mathrm{eff,p}}\frac{\partial^2 c}{\partial x^2}+(1-t_+)a_{\mathrm{p}}j_p$$

$$\sigma_{\mathrm{eff,p}}\frac{\partial^2\Phi_1}{\partial x^2}=a_{\mathrm{p}}Fj_p$$

$$-\frac{\partial}{\partial x}\left(\kappa_{\mathrm{eff,p}}\frac{\partial\Phi_2}{\partial x}\right)+\beta\frac{\partial}{\partial x}\left(\mathrm{eff,p}\frac{\partial\ln c}{\partial x}\right)=a_{\mathrm{p}}Fj_p$$

- Negative Electrode:

$$\frac{\partial c_{s,n}(r,t)}{\partial t}=D_{s,n}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial c_{s,n}(r,t)}{\partial r}\right)$$

$$\varepsilon_{\mathrm{n}}\frac{\partial c}{\partial t}=D_{\mathrm{eff,n}}\frac{\partial^2 c}{\partial x^2}+(1-t_+)a_{\mathrm{n}}j_n$$

$$\sigma_{\mathrm{eff,n}}\frac{\partial^2\Phi_1}{\partial x^2}=a_{\mathrm{n}}Fj_n$$

$$-\frac{\partial}{\partial x}\left(\kappa_{\mathrm{eff,n}}\frac{\partial\Phi_2}{\partial x}\right)+\beta\frac{\partial}{\partial x}\left(\mathrm{eff,n}\frac{\partial\ln c}{\partial x}\right)=a_{\mathrm{n}}Fj_n$$

- Separator:

$$\varepsilon_{\mathrm{s}}\frac{\partial c}{\partial t}=D_{\mathrm{eff,s}}\frac{\partial^2 c}{\partial x^2}$$

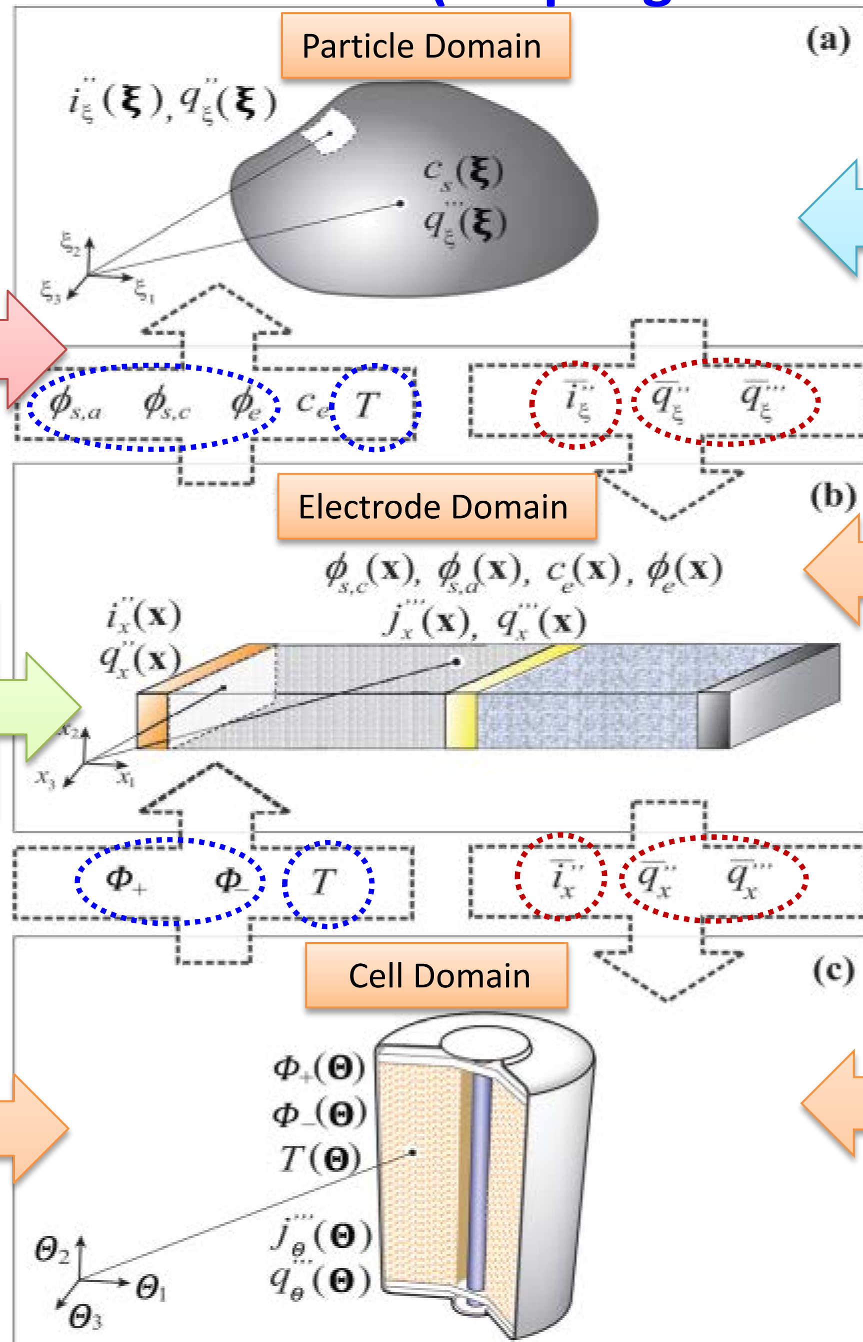
$$-\frac{\partial}{\partial x}\left(\kappa_{\mathrm{eff,s}}\frac{\partial\Phi_2}{\partial x}\right)+\beta\frac{\partial}{\partial x}\left(\mathrm{eff,s}\frac{\partial\ln c}{\partial x}\right)=0$$

- BV: $j_i=2k_i\left(c_{s,\mathrm{max,i}}-c_s(R_{s,i})\right)^{0.5}c_s(R_{s,i})^{0.5}c^{0.5}\sinh\left[\frac{0.5F}{RT}(\Phi_1-\Phi_2-U_i)\right]$

MSMD Model (coupling between inter-domains)

T, temperatures are from the cell level domain. No energy equations in the electrode and the particle domain

Current is generated from the particle level and applied for the electrode and the cell domain



Heat source is generated from the particle level (heat of charge transfer and mixing)

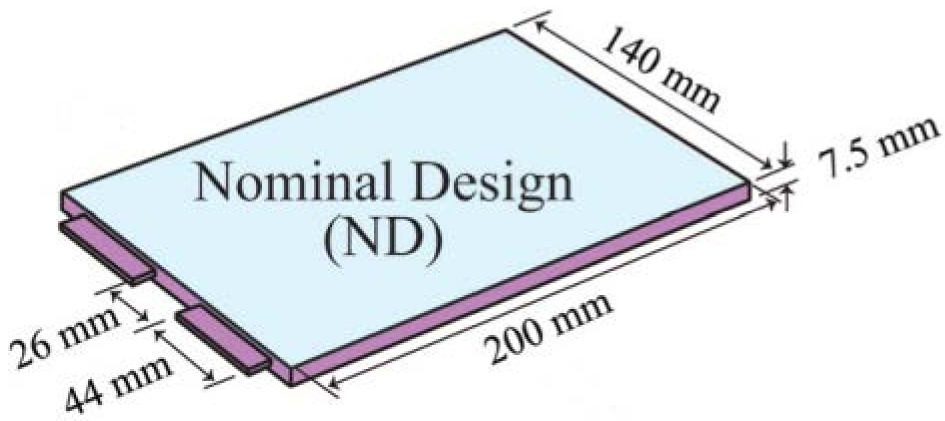
Φ_+ and Φ_- provide to the electrode to compute potentials in the electrode interfaces

Φ_+ and Φ_- are the potential at the positive and the negative current collectors

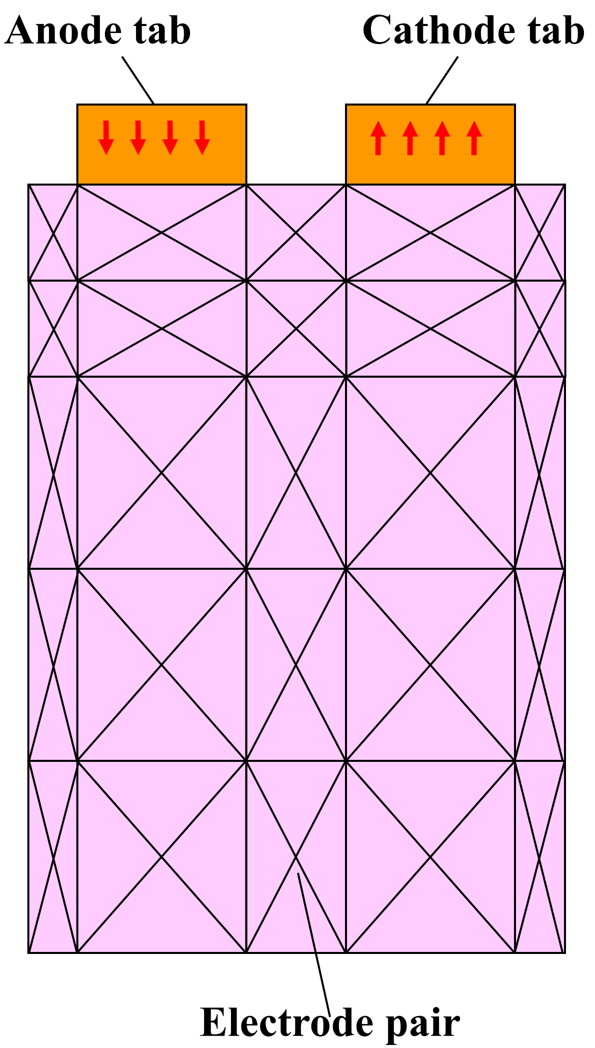
Heat source is also added in the electrode region by contact resistance and others

20-Ah LG Normal Design cell

Modeling with finite element method



Real cell*

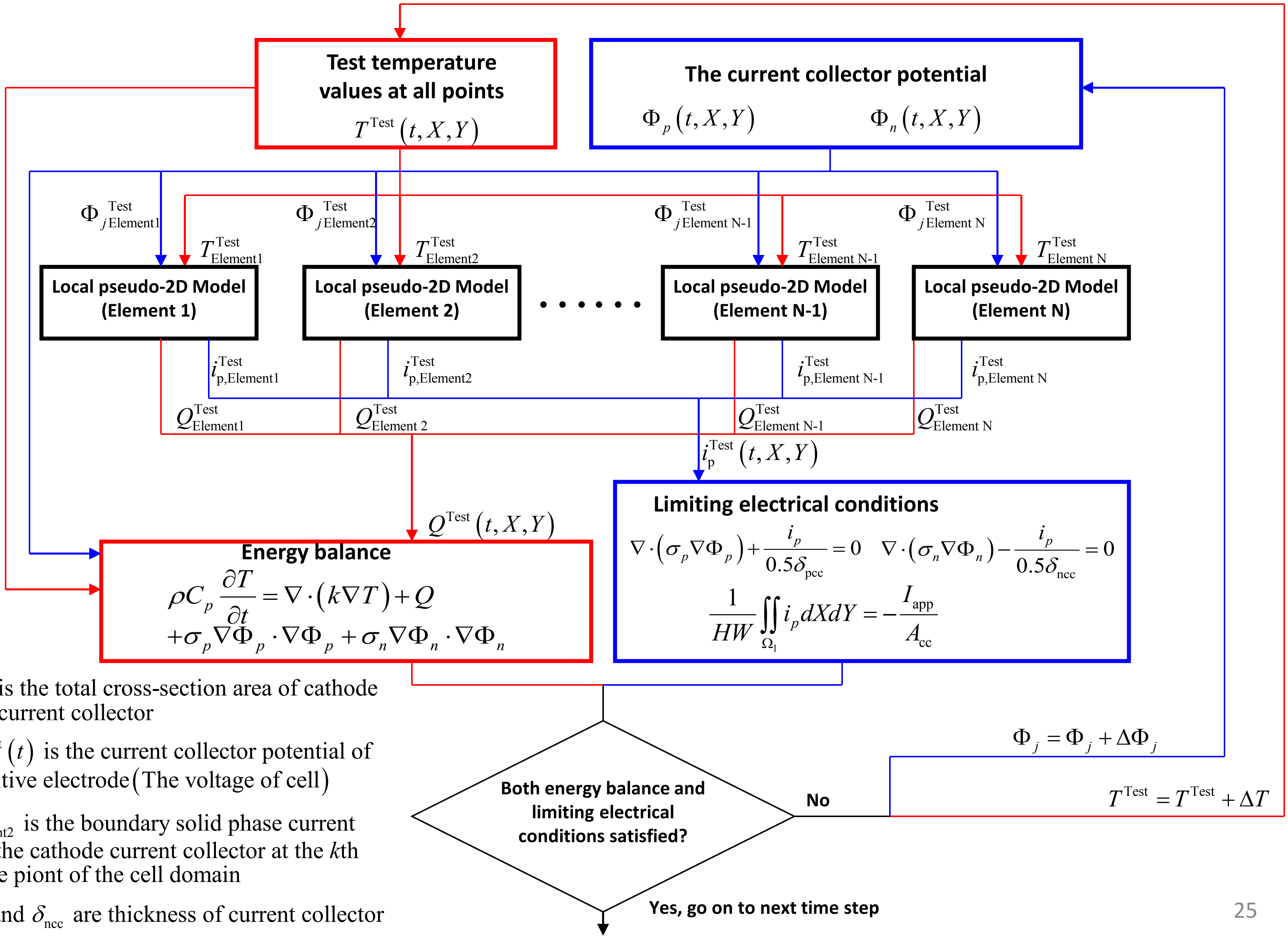


Model domain

*Gi-Heon Kim,z Kandler Smith,Kyu-Jin Lee, Shriram Santhanagopalan, and Ahmad Pesaran, Journal of The Electrochemical Society, 158 (8) A955-A969 (2011)

ESim LLC

Flowchart for distributed pseudo-2D thermal model



A_{cc} is the total cross-section area of cathode current collector

$V_{\text{cell}}^{\text{Test}}(t)$ is the current collector potential of positive electrode (The voltage of cell)

$i_{\text{p,Point2}}^{\text{Test}}$ is the boundary solid phase current for the cathode current collector at the kth node piont of the cell domain

δ_{pcc} and δ_{ncc} are thickness of current collector

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20-Ah LG Normal Design cell

- **Anode initial SOC: 0.63**
- **Cathode Initial SOC: 0.41**
- **End of discharge voltage: 2.5V**